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## 13. ABSTRACT (Maximum 200 words)

Theoretical studies of the interaction of charged particles and electromagnetic radiation with matter have been performed. Particular emphasis has been given to ionizing radiation and the details of energy deposition by the radiation. New phenomena have been discovered in the area of ionization in ion-atom and atom-atom collisions. Models of electron impact ionization of atoms and molecules have been extended to the relativistic range. In addition, relativistic effects in the photoionization of very heavy atoms and ions have been delineated in detail for the first time. Finally, a number of investigations of various aspects of photoionization of excited atoms have been carried out which have given new insight into the process, both for outer and inner shell ionization. Of particular interest is the discovery that inner shell photoionization of excited atoms is primarily a many-body process.

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INVESTIGATIONS OF THE INTERACTIONS  
OF RADIATION WITH MATTER

FINAL REPORT

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During the period of this contract from the U.S. Army Research Office, our theoretical research in atomic and molecular physics has proceeded well. In this report, the principal areas of investigation are briefly discussed with the progress made in each area highlighted. The results of the calculations provide further insight into the basic nature of these fundamental atomic processes which are important input data for plasma physics, atmospheric, solar, and astrophysics, radiation physics and therapy, for surface studies and catalysis, for studies of the transport of energy from the site of thermonuclear reaction, for energy-loss electron microscopy, for the production of a nuclear-pumped or x-ray laser, for generation and detection of centimeter wavelengths, and for the passage of particle, UV, or x-ray beams through the atmosphere. The report is as non-technical as possible; numerous references are given to published works where the technical details can be found. In addition, a complete listing of the 22 publications resulting from this work is presented in the appendix.

## I. INTERACTION OF CHARGED PARTICLES WITH MATTER

A major step in this area has dealt with electron ejection in ion-atom collisions where the ion brings along its own electrons. We have considered  $\text{He}^+ + \text{He}/\text{Ar}$  collisions<sup>1</sup>, since experimental data was available, and we were able to predict the total ejected electron energy (and angular) distribution rather well. The calculation considered electron ejection by both target and projectile so that we were able to delineate which part of the electron distribution came from the target and which came from the projectile; this was not yet available experimentally since the breakdown required a coincidence experiment. From this work, we also learned the importance of the ejection of an electron by one particle and the simultaneous excitation or ionization of the other.

In addition, based upon these results, we have made predictions that electron ejection plus simultaneous excitation should dominate the neutral-neutral collision process, and that prediction has been confirmed.<sup>2</sup> This work showed that simultaneous ionization was also the dominant process in projectile ionization by neutral targets.

We have also made considerable progress in the semi-empirical modelling of electron ejection ( $\delta$ -ray) cross sections in ion (electron)-atom (molecule) collisions with a view to extending existing data. The model is based generally on the Bethe expansion of the cross section at high impact energies.<sup>3</sup> The leading term in this expansion is related to the photoionization cross section for which there exists significantly more reliable experimental data than for electron ejection cross sections. In the past, have had substantial success applying this technique to protons on atoms,<sup>4</sup> protons on molecules<sup>5</sup>, electrons on atoms<sup>4,6</sup> and electrons on molecules.<sup>7</sup> In this work, we have extended the formulation to include relativistic effects so that we can now deal with very energetic collisions.<sup>8</sup>

## II. INTERACTION OF ELECTROMAGNETIC RADIATION WITH MATTER

In the area of relativistic effects our primary goal has been to understand in what ways the non-relativistic photoabsorption results are modified by relativistic interactions and to ascertain the underlying cause(s) of these modifications. Owing to the paucity of experimental results, we have been unable to compare our predictions base on simple relativistic calculations with measurements. Thus, to provide some check, we have performed a number of calculations at the sophisticated relativistic-random-phase approximation (RRPA) level.<sup>9</sup> In particular, we have performed a major study of the photoionization of all of the outer subshells of the high-Z

Rn( $Z=86$ ) and Ra( $Z=88$ ) atoms.<sup>10</sup> In this work, we have uncovered a variety of new phenomena owing to the interplay between relativistic and correlation effects; these phenomena include correlation induced minima and relativistically split minima which dominate the spectral distribution of oscillator strength in the near threshold region.

We have also applied the RRPA to the photoionization of positive ions of the Mg and Ar isonuclear sequences<sup>11</sup> and found that the resulting inner shell cross sections showed the characteristic independence on the removal of outer shell electrons predicted by less sophisticated calculations.<sup>12</sup> This confirms the utility of the procedure of transferring cross sections of neutral atoms, where data is relatively plentiful, to ions where data is far more sparse.

In the area of excited state photoabsorption, we have completed a number of studies. We have verified that our calculations are of such quality to give excellent agreement with experiment for two separate excited states in cesium.<sup>13,14</sup> We have also learned some new phenomenology concerning shape resonances in the photoionization of excited states of high  $Z$  atoms.<sup>15</sup> In addition, in conjunction with an experimental group, we have uncovered new phenomenology in the photoionization of Rydberg atoms very very close to threshold.<sup>16</sup> Furthermore, we have laid to rest a controversy regarding the photoionization of the first excited state of the Ba atom.<sup>17</sup> And we have discovered a new phenomenon in the inner shell photoionization of excited states;<sup>18</sup> basically, we have found that, in such processes, the overwhelmingly dominant transitions are ionization plus excitation, often called shake-up. This was explained in terms of the relaxation of the excited electron under the action of the removal of an inner shell electron which changes the screening dramatically.

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